Butanedioic acid, hydroxy-, dimethyl ester

Other names:	Malic acid, dimethyl ester
	Dimethyl malate
	DL-Malic acid, dimethyl ester
Inchi:	InChI=1S/C6H10O5/c1-10-5(8)3-4(7)6(9)11-2/h4,7H,3H2,1-2H3
InchiKey:	YSEKNCXYRGKTBJ-UHFFFAOYSA-N
Formula:	C6H10O5
SMILES:	COC(=O)CC(O)C(=O)OC
Mol. weight [g/mol]:	162.14
CAS:	1587-15-1

Physical Properties

Property code	Value	Unit	Source
gf	-607.46	kJ/mol	Joback Method
hf	-814.28	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	63.55	kJ/mol	Joback Method
log10ws	0.57		Crippen Method
logp	-0.917		Crippen Method
mcvol	116.150	ml/mol	McGowan Method
pc	3896.50	kPa	Joback Method
rinpol	1125.90		NIST Webbook
rinpol	1125.90		NIST Webbook
tb	581.00	K	Joback Method
tc	763.03	K	Joback Method
tf	347.52	K	Joback Method
vc	0.432	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	280.03	J/mol×K	581.00	Joback Method
cpg	318.69	J/mol×K	732.69	Joback Method
cpg	311.67	J/mol×K	702.35	Joback Method
cpg	304.29	J/mol×K	672.01	Joback Method

cpg	296.55	J/mol×K	641.68	Joback Method
cpg	288.46	J/mol×K	611.34	Joback Method
cpg	325.33	J/mol×K	763.03	Joback Method
dvisc	0.0000920	Pa×s	581.00	Joback Method
dvisc	0.0001396	Pa×s	542.09	Joback Method
dvisc	0.0002257	Pa×s	503.17	Joback Method
dvisc	0.0003956	Pa×s	464.26	Joback Method
dvisc	0.0007685	Pa×s	425.35	Joback Method
dvisc	0.0017064	Pa×s	386.43	Joback Method
dvisc	0.0045299	Pa×s	347.52	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1587151&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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